Peridynamics as an upscaling of Molecular Dynamics

Pablo Seleson[*,‡], Michael L. Parks[†,‡], and Max Gunzburger [*]

Peridynamics, an alternative model of continuum mechanics, was introduced in [2], where an integral formulation is presented. Peridynamics is a nonlocal model, accounting for the effects of long-range forces. Certain quadrature-based discretizations of peridynamics have similar computational structure to molecular dynamics, as both methods compute the forces on a particle by summing the forces from surrounding particles. This allows a straightforward implementation of peridynamics within existing molecular dynamics codes [1].

We overview current peridynamic computational capabilities, then explore how the peridynamic model can be cast as an upscaling of molecular dynamics by matching nonlocal molecular dynamics models with peridynamics, and comparing their dispersion relations.

References

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[*]Dept. of Scientific Computing, 400 Dirac Science Library, Florida State University, Tallahassee, FL 32306-4120. Research supported by DOE/OASCR.

[†]Computational Mathematics and Algorithms, Sandia National Laboratories, P.O. Box 5800, Albuquerque, NM 87185-1320. Research supported by DOE/OASCR.

[‡]Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94AL85000.